

1,3-Benzodioxole-5-methanol
495-76-1 | DTXSID3060089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.25 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.02e-01

Confidence level: 6.45e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethanol, 2-(phenylamino)-</div> <div>Measured: 3.34e-01</div> <div>Predicted: 8.15e-01</div>	<div>Image not found</div> <div>Noxytiolin [INN:BAN:DCF]</div> <div>Measured: 8.32e-01</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>2-Amino-2-ethyl-1,3-propanediol</div> <div>Measured: 8.39</div> <div>Predicted: 7.55</div>
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